

A new polymorph of 1,3-bis(pentafluorophenyl)urea

Tsunehisa Okuno

Department of Material Science and Chemistry, Wakayama University, Sakaedani, Wakayama, 640-8510, Japan

Correspondence e-mail: okuno@center.wakayama-u.ac.jp

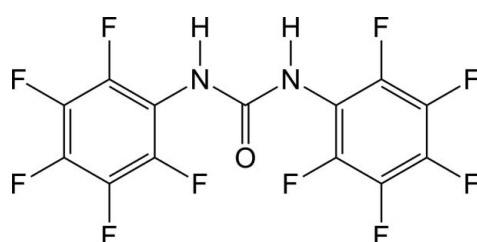
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Key indicators: single-crystal X-ray study; $T = 93\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$; R factor = 0.031; wR factor = 0.080; data-to-parameter ratio = 8.3.

The title compound, $\text{C}_{13}\text{H}_2\text{F}_{10}\text{N}_2\text{O}$, has been previously described in the space group $Pbca$ with $Z = 8$ [Jai-nhuknan *et al.* (1997). *Acta Cryst. C* **53**, 455–457]. The current $P2_12_12_1$ polymorph was obtained from a tetrahydrofuran solution. The pentafluorophenyl rings make dihedral angles of 50.35 (6) and 54.94 (6) $^\circ$ with the urea fragment, in close accord with those reported for the first polymorph. In the crystal, both of the N–H groups donate H atoms to the same carbonyl O atom, forming a one-dimensional molecular array along the a axis. There are close contacts between perfluorophenyl C atoms within the array [$3.228(3)\text{ \AA}$] and halogen bonds are also observed between the arrays [$\text{F} \cdots \text{F} = 2.709(2)$ and $2.7323(18)\text{ \AA}$].

Related literature

For the structure of the first reported polymorph, see: Jai-nhuknan *et al.* (1997). For the related structure of 1,3-diphenylurea, see: Dannecker *et al.* (1979). For background to organofluorine chemistry, see: Chambers (2004).



Experimental

Crystal data

$\text{C}_{13}\text{H}_2\text{F}_{10}\text{N}_2\text{O}$	$V = 1273.1(4)\text{ \AA}^3$
$M_r = 392.16$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 4.5798(7)\text{ \AA}$	$\mu = 0.23\text{ mm}^{-1}$
$b = 9.5411(16)\text{ \AA}$	$T = 93\text{ K}$
$c = 29.136(5)\text{ \AA}$	$0.15 \times 0.15 \times 0.03\text{ mm}$

Data collection

Rigaku Saturn724+ diffractometer	10307 measured reflections
Absorption correction: numerical (<i>NUMABS</i> ; Rigaku, 1999)	1993 independent reflections
$T_{\min} = 0.978$, $T_{\max} = 0.993$	1941 reflections with $F^2 > 2\sigma(F^2)$
	$R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$	2 restraints
$wR(F^2) = 0.080$	Only H-atom coordinates refined
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.34\text{ e \AA}^{-3}$
1991 reflections	$\Delta\rho_{\text{min}} = -0.20\text{ e \AA}^{-3}$
241 parameters	

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
N1–H1 \cdots O1 ⁱ	0.864 (18)	2.057 (18)	2.850 (3)	152 (3)
N2–H2 \cdots O1 ⁱ	0.879 (18)	2.008 (18)	2.825 (3)	154 (3)

Symmetry code: (i) $x + 1, y, z$.

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR92* (Altomare, *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2101).

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supplementary materials

Acta Cryst. (2013). E69, o608 [doi:10.1107/S1600536813007836]

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Comment

Perfluoro aromatic compounds have attracted interest from the viewpoint of the electronic and structural comparison with the original compounds (Chambers, 2004). The title compound, (I), is a perfluoro compound of 1,3-diphenylurea (Dannecker *et al.*, 1979). Previously, (I) was isolated in an orthorhombic *Pbca* polymorph with $Z = 8$ [Jai-nhuknan *et al.*, 1997]. A new orthorhombic *P2₁2₁2₁* polymorph was obtained by recrystallization from a tetrahydrofuran solution.

The dihedral angle between the C1—C6/F1—F5 (r.m.s. deviation = 0.0223 Å) and the C7—C12/F6—F10 (r.m.s. deviation = 0.0181 Å) pentafluorophenyl rings is 30.93 (3)°, which is smaller than that of the reported polymorph. The pentafluorophenyl rings make dihedral angles of 50.35 (6)° and 54.94 (6)°, respectively, with the C13/N1/N2/O1 urea fragment (r.m.s. deviation = 0.0011 Å), and this situation is almost accordance with the reported polymorph.

Both of the N—H groups in one molecule donate protons to the same carbonyl O atom, forming a one-dimensional molecular array along the α axis, where the N···O distances were 2.850 (3) Å for N1···O1ⁱ and 2.825 (3) Å for N2···O1ⁱ [Symmetry code: (i) $x + 1, y, z$] (Figure 2). There are close contacts between perfluorophenyl carbons within the array, where the C2···C5ⁱ distance is 3.228 (3) Å. Halogen-bonds are also recognized between the arrays. The distances of F2···F10ⁱⁱ and F1···F5ⁱⁱⁱ are 2.709 (2) Å and 2.7323 (18) Å, respectively [Symmetry codes: (ii) $-x + 1, y + 1/2, -z + 1/2$ (iii) $x + 2, y + 1/2, -z + 1/2$.] (Figure 2).

Experimental

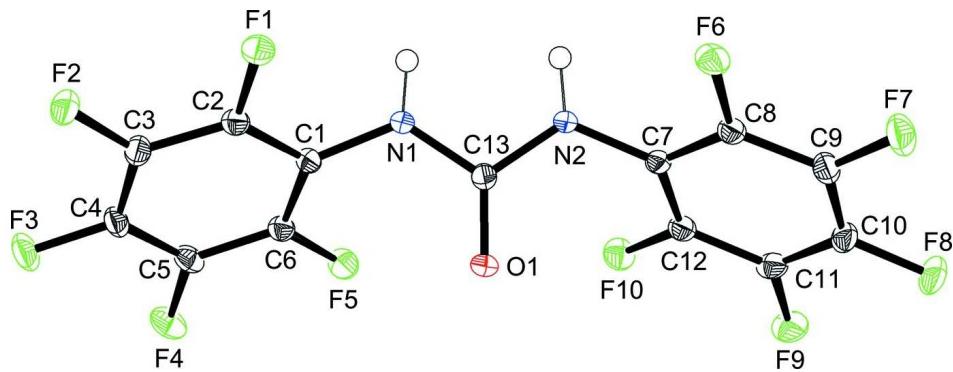
The title compound was commercially purchased and recrystallized from a tetrahydrofuran solution.

Refinement

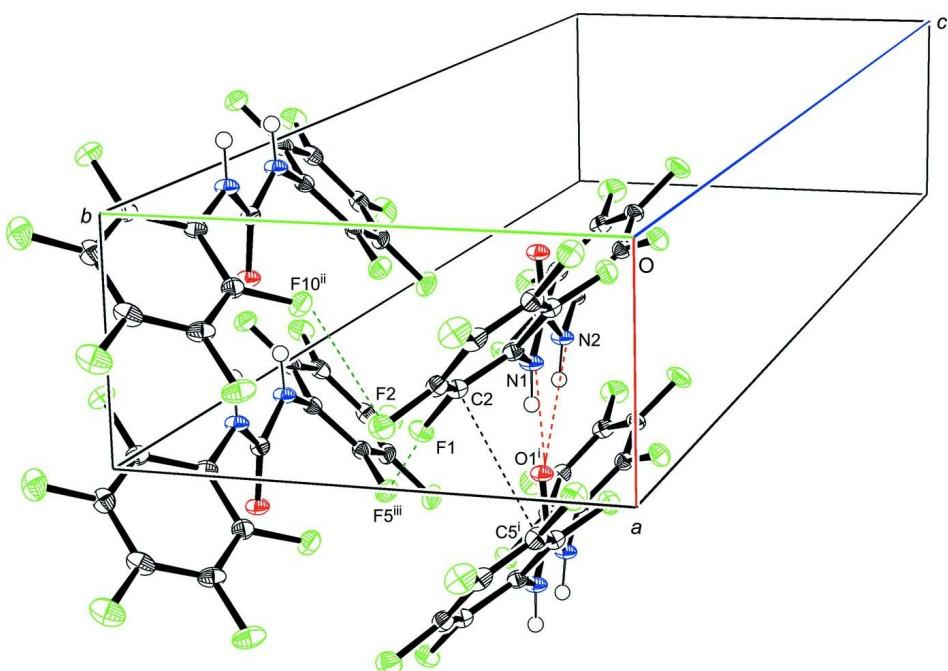
Friedel pairs were merged because the molecule itself was achiral and because there were not any anomalous scattering effects. The N-bound H atom was obtained from a difference Fourier map and was refined isotropically with the restriction of N—H range between 0.85 Å and 0.89 Å. $U_{\text{iso}}(\text{H})$ values of the H atoms were set at 1.2 U_{eq} (parent atom).

Computing details

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear* (Rigaku, 2008); data reduction: *CrystalClear* (Rigaku, 2008); program(s) used to solve structure: *SIR92* (Altomare, *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2010).

**Figure 1**

The asymmetric unit of the title compound with atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres.

**Figure 2**

A view of the intermolecular interactions in the title compound. [Symmetry codes: (i) $x + 1, y, z$ (ii) $-x + 1, y + 1/2, -z + 1/2$ (iii) $-x + 2, y + 1/2, -z + 1/2$.]

1,3-Bis(pentafluorophenyl)urea

Crystal data

$C_{13}H_2F_{10}N_2O$

$M_r = 392.16$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 4.5798 (7) \text{ \AA}$

$b = 9.5411 (16) \text{ \AA}$

$c = 29.136 (5) \text{ \AA}$

$V = 1273.1 (4) \text{ \AA}^3$

$Z = 4$

$F(000) = 768.00$

$D_x = 2.046 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71075 \text{ \AA}$

Cell parameters from 4650 reflections

$\theta = 2.3\text{--}31.2^\circ$

$\mu = 0.23 \text{ mm}^{-1}$

$T = 93 \text{ K}$

Platelet, colorless

$0.15 \times 0.15 \times 0.03 \text{ mm}$

Data collection

Rigaku Saturn724+
diffractometer
Detector resolution: 28.445 pixels mm⁻¹
 ω scans
Absorption correction: numerical
(NUMABS; Rigaku, 1999)
 $T_{\min} = 0.978$, $T_{\max} = 0.993$
10307 measured reflections

1993 independent reflections
1941 reflections with $F^2 > 2\sigma(F^2)$
 $R_{\text{int}} = 0.023$
 $\theta_{\text{max}} = 29.0^\circ$
 $h = -6 \rightarrow 5$
 $k = -12 \rightarrow 13$
 $l = -39 \rightarrow 37$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.080$
 $S = 1.09$
1991 reflections
241 parameters
2 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
Only H-atom coordinates refined
 $w = 1/[\sigma^2(F_o^2) + (0.0393P)^2 + 0.6807P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.34 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.20 \text{ e } \text{\AA}^{-3}$

*Special details***Geometry.** ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement was performed using all reflections except for two with very negative F^2 . The weighted R -factor (wR) and goodness of fit (S) are based on F^2 . R -factor (gt) are based on F . The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating R -factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	1.1418 (3)	0.61873 (13)	0.20307 (4)	0.0201 (3)
F2	0.9729 (3)	0.60115 (14)	0.11485 (4)	0.0230 (3)
F3	0.5296 (4)	0.42251 (14)	0.09057 (4)	0.0261 (3)
F4	0.2849 (3)	0.25518 (13)	0.15527 (4)	0.0235 (3)
F5	0.4741 (3)	0.26032 (12)	0.24218 (4)	0.0199 (3)
F6	1.1205 (3)	0.65289 (13)	0.41004 (4)	0.0209 (3)
F7	0.9048 (4)	0.66890 (14)	0.49612 (4)	0.0269 (3)
F8	0.4722 (4)	0.49024 (15)	0.52340 (4)	0.0286 (3)
F9	0.2803 (3)	0.28817 (15)	0.46530 (4)	0.0261 (3)
F10	0.5071 (3)	0.26629 (12)	0.38011 (4)	0.0213 (3)
O1	0.4972 (3)	0.46701 (15)	0.30935 (5)	0.0163 (3)
N1	0.9286 (4)	0.4477 (2)	0.27009 (5)	0.0154 (3)
N2	0.9324 (4)	0.45284 (19)	0.34806 (5)	0.0149 (3)
C1	0.8112 (5)	0.4427 (2)	0.22555 (6)	0.0143 (4)
C2	0.9298 (5)	0.5288 (2)	0.19172 (6)	0.0156 (4)
C3	0.8433 (5)	0.5207 (2)	0.14616 (6)	0.0172 (4)
C4	0.6225 (5)	0.4295 (3)	0.13398 (6)	0.0180 (4)
C5	0.4991 (5)	0.3442 (2)	0.16699 (6)	0.0170 (4)
C6	0.5947 (5)	0.3492 (2)	0.21201 (6)	0.0150 (4)
C7	0.8117 (4)	0.4624 (2)	0.39231 (6)	0.0141 (4)
C8	0.9103 (5)	0.5630 (2)	0.42307 (6)	0.0155 (4)

C9	0.8013 (5)	0.5723 (2)	0.46721 (6)	0.0181 (4)
C10	0.5852 (5)	0.4809 (3)	0.48127 (6)	0.0196 (4)
C11	0.4853 (5)	0.3785 (2)	0.45158 (6)	0.0184 (4)
C12	0.6005 (5)	0.3694 (2)	0.40767 (6)	0.0158 (4)
C13	0.7652 (5)	0.4563 (2)	0.30915 (6)	0.0139 (4)
H1	1.117 (4)	0.451 (3)	0.2722 (9)	0.0184*
H2	1.123 (4)	0.459 (3)	0.3452 (9)	0.0179*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0170 (6)	0.0229 (6)	0.0204 (6)	-0.0048 (5)	-0.0003 (5)	-0.0012 (5)
F2	0.0234 (6)	0.0297 (6)	0.0158 (5)	0.0024 (6)	0.0033 (5)	0.0049 (5)
F3	0.0296 (7)	0.0353 (7)	0.0135 (5)	0.0054 (7)	-0.0075 (6)	-0.0045 (5)
F4	0.0220 (6)	0.0210 (6)	0.0276 (6)	-0.0030 (6)	-0.0094 (6)	-0.0061 (5)
F5	0.0200 (6)	0.0195 (6)	0.0202 (6)	-0.0027 (6)	-0.0016 (5)	0.0030 (5)
F6	0.0185 (6)	0.0226 (6)	0.0215 (6)	-0.0072 (6)	-0.0018 (5)	0.0029 (5)
F7	0.0326 (8)	0.0299 (7)	0.0181 (5)	-0.0002 (7)	-0.0049 (6)	-0.0073 (5)
F8	0.0303 (7)	0.0426 (8)	0.0129 (5)	0.0047 (7)	0.0060 (6)	0.0026 (5)
F9	0.0201 (6)	0.0324 (7)	0.0259 (6)	-0.0066 (6)	0.0043 (6)	0.0104 (6)
F10	0.0221 (6)	0.0197 (6)	0.0221 (6)	-0.0056 (6)	-0.0011 (5)	-0.0017 (5)
O1	0.0100 (6)	0.0234 (7)	0.0154 (6)	-0.0001 (6)	-0.0011 (6)	0.0006 (6)
N1	0.0097 (7)	0.0242 (8)	0.0122 (7)	0.0003 (7)	-0.0006 (6)	-0.0007 (6)
N2	0.0094 (7)	0.0237 (8)	0.0117 (7)	0.0000 (7)	-0.0004 (6)	0.0004 (6)
C1	0.0126 (8)	0.0174 (8)	0.0129 (8)	0.0016 (8)	-0.0009 (7)	-0.0011 (7)
C2	0.0134 (8)	0.0178 (8)	0.0155 (8)	0.0009 (7)	-0.0004 (7)	-0.0017 (7)
C3	0.0180 (9)	0.0202 (9)	0.0135 (8)	0.0046 (8)	0.0014 (7)	0.0013 (7)
C4	0.0193 (9)	0.0230 (9)	0.0116 (8)	0.0063 (9)	-0.0036 (8)	-0.0040 (7)
C5	0.0159 (9)	0.0165 (8)	0.0186 (8)	0.0001 (8)	-0.0051 (8)	-0.0043 (7)
C6	0.0136 (8)	0.0163 (8)	0.0152 (8)	0.0015 (8)	-0.0007 (7)	-0.0010 (7)
C7	0.0111 (8)	0.0184 (9)	0.0127 (8)	0.0013 (8)	-0.0003 (7)	0.0026 (7)
C8	0.0134 (8)	0.0180 (8)	0.0151 (8)	-0.0005 (8)	-0.0008 (7)	0.0026 (7)
C9	0.0197 (9)	0.0200 (9)	0.0147 (8)	0.0027 (8)	-0.0029 (8)	-0.0017 (7)
C10	0.0190 (9)	0.0277 (10)	0.0122 (8)	0.0060 (9)	0.0015 (7)	0.0032 (7)
C11	0.0141 (8)	0.0224 (9)	0.0188 (8)	0.0003 (8)	0.0015 (8)	0.0081 (7)
C12	0.0139 (8)	0.0172 (8)	0.0162 (8)	0.0003 (8)	-0.0012 (7)	0.0010 (7)
C13	0.0141 (8)	0.0150 (8)	0.0126 (8)	-0.0006 (7)	-0.0003 (7)	0.0000 (7)

Geometric parameters (\AA , ^\circ)

F1—C2	1.337 (3)	C1—C2	1.393 (3)
F2—C3	1.332 (3)	C1—C6	1.391 (3)
F3—C4	1.336 (3)	C2—C3	1.387 (3)
F4—C5	1.342 (3)	C3—C4	1.380 (3)
F5—C6	1.340 (3)	C4—C5	1.381 (3)
F6—C8	1.344 (3)	C5—C6	1.384 (3)
F7—C9	1.336 (3)	C7—C8	1.389 (3)
F8—C10	1.335 (3)	C7—C12	1.387 (3)
F9—C11	1.336 (3)	C8—C9	1.382 (3)
F10—C12	1.340 (3)	C9—C10	1.381 (3)

O1—C13	1.232 (3)	C10—C11	1.383 (3)
N1—C1	1.405 (3)	C11—C12	1.387 (3)
N1—C13	1.364 (3)	N1—H1	0.864 (18)
N2—C7	1.406 (3)	N2—H2	0.879 (18)
N2—C13	1.368 (3)		
F1···F2	2.6895 (18)	F9···C1 ^{xiv}	3.197 (3)
F1···N1	2.725 (2)	F10···F1 ^{vi}	3.2313 (18)
F2···F3	2.744 (2)	F10···F2 ^{viii}	2.709 (2)
F3···F4	2.7126 (18)	F10···F2 ^{vi}	2.859 (2)
F4···F5	2.6767 (18)	F10···F3 ^{viii}	3.3936 (19)
F5···O1	2.7803 (19)	F10···N2 ^v	3.312 (3)
F5···N1	2.862 (3)	F10···C3 ^{viii}	2.942 (3)
F5···C13	3.014 (3)	F10···C4 ^{viii}	3.293 (3)
F6···F7	2.6999 (18)	O1···F4 ⁱ	3.101 (2)
F6···N2	2.765 (2)	O1···F5 ⁱ	3.1785 (19)
F7···F8	2.732 (2)	O1···N1 ^v	2.850 (3)
F8···F9	2.712 (2)	O1···N2 ^v	2.825 (3)
F9···F10	2.6989 (18)	O1···C13 ^v	3.354 (3)
F10···O1	2.8143 (19)	N1···F1 ^{vi}	3.251 (3)
F10···N2	2.799 (3)	N1···F5 ⁱⁱⁱ	3.178 (3)
F10···C13	2.993 (3)	N1···F5 ⁱ	3.525 (3)
O1···C1	2.843 (3)	N1···O1 ⁱⁱⁱ	2.850 (3)
O1···C6	3.083 (3)	N2···F1 ^{vi}	3.535 (3)
O1···C7	2.814 (3)	N2···F2 ^{vi}	3.552 (3)
O1···C12	3.049 (3)	N2···F4 ⁱ	3.053 (3)
C1···C4	2.807 (3)	N2···F10 ⁱⁱⁱ	3.312 (3)
C2···C5	2.741 (3)	N2···O1 ⁱⁱⁱ	2.825 (3)
C2···C13	3.571 (3)	C1···F1 ^v	3.557 (3)
C3···C6	2.767 (3)	C1···F4 ⁱⁱⁱ	3.478 (3)
C6···C13	3.109 (3)	C1···F5 ⁱⁱⁱ	3.532 (3)
C7···C10	2.797 (3)	C1···F5 ⁱ	3.432 (3)
C8···C11	2.753 (3)	C2···F4 ⁱⁱⁱ	3.254 (3)
C8···C13	3.535 (3)	C2···F5 ⁱ	3.466 (3)
C9···C12	2.757 (3)	C2···C5 ⁱⁱⁱ	3.228 (3)
C12···C13	3.082 (3)	C2···C6 ⁱⁱⁱ	3.544 (3)
F1···F5 ⁱ	3.5106 (18)	C3···F4 ⁱⁱⁱ	3.252 (3)
F1···F5 ⁱⁱ	2.7323 (18)	C3···F10 ⁱ	2.942 (3)
F1···F10 ⁱⁱ	3.2313 (18)	C3···C5 ⁱⁱⁱ	3.496 (3)
F1···N1 ⁱⁱ	3.251 (3)	C4···F1 ^v	3.487 (3)
F1···N2 ⁱⁱ	3.535 (3)	C4···F2 ^v	3.441 (3)
F1···C1 ⁱⁱⁱ	3.557 (3)	C4···F4 ⁱⁱⁱ	3.515 (3)
F1···C4 ⁱⁱⁱ	3.487 (3)	C4···F6 ^{vi}	3.162 (3)
F1···C5 ⁱⁱⁱ	3.263 (3)	C4···F10 ⁱ	3.293 (3)
F1···C6 ⁱⁱⁱ	3.315 (3)	C5···F1 ^v	3.263 (3)
F1···C6 ⁱⁱ	3.523 (3)	C5···F6 ^{vi}	3.377 (3)
F1···C13 ⁱⁱ	3.269 (3)	C5···C2 ^v	3.228 (3)
F2···F3 ⁱⁱⁱ	3.147 (2)	C5···C3 ^v	3.496 (3)
F2···F8 ^{iv}	2.8148 (18)	C6···F1 ^v	3.315 (3)

F2···F9 ⁱ	3.1594 (19)	C6···F1 ^{vi}	3.523 (3)
F2···F10 ⁱ	2.709 (2)	C6···C2 ^v	3.544 (3)
F2···F10 ⁱⁱ	2.859 (2)	C7···F2 ^{vi}	3.591 (3)
F2···N2 ⁱⁱ	3.552 (3)	C7···F4 ⁱ	3.150 (3)
F2···C4 ⁱⁱⁱ	3.441 (3)	C7···F9 ⁱⁱⁱ	3.448 (3)
F2···C7 ⁱⁱ	3.591 (3)	C8···F4 ⁱ	3.061 (3)
F2···C12 ⁱⁱ	3.286 (3)	C8···F9 ⁱⁱⁱ	3.356 (3)
F3···F2 ^v	3.147 (2)	C8···C11 ⁱⁱⁱ	3.275 (3)
F3···F6 ^{vi}	3.0309 (19)	C9···F7 ^{xi}	3.246 (3)
F3···F7 ^{iv}	2.9024 (18)	C9···F8 ⁱⁱⁱ	3.568 (3)
F3···F8 ^{vii}	3.131 (2)	C9···F9 ⁱⁱⁱ	3.487 (3)
F3···F8 ^{iv}	3.119 (2)	C10···F6 ^v	3.395 (3)
F3···F10 ⁱ	3.3936 (19)	C10···F7 ^{xi}	3.504 (3)
F4···F6 ^{viii}	2.8319 (18)	C10···F9 ^{xiii}	3.133 (3)
F4···F6 ^{vi}	3.4627 (19)	C11···F6 ^v	3.333 (3)
F4···O1 ^{viii}	3.101 (2)	C11···F9 ^{xiii}	3.197 (3)
F4···N2 ^{viii}	3.053 (3)	C11···C8 ^v	3.275 (3)
F4···C1 ^v	3.478 (3)	C12···F2 ^{vi}	3.286 (3)
F4···C2 ^v	3.254 (3)	C12···F6 ^v	3.486 (3)
F4···C3 ^v	3.252 (3)	C13···F1 ^{vi}	3.269 (3)
F4···C4 ^v	3.515 (3)	C13···F4 ⁱ	3.043 (3)
F4···C7 ^{viii}	3.150 (3)	C13···F5 ⁱ	3.442 (3)
F4···C8 ^{viii}	3.061 (3)	C13···O1 ⁱⁱⁱ	3.354 (3)
F4···C13 ^{viii}	3.043 (3)	F1···H1	2.58 (3)
F5···F1 ^{viii}	3.5106 (18)	F5···H1	3.57 (2)
F5···F1 ^{vi}	2.7323 (18)	F6···H2	2.64 (3)
F5···O1 ^{viii}	3.1785 (19)	F10···H2	3.52 (3)
F5···N1 ^v	3.178 (3)	O1···H1	3.040 (19)
F5···N1 ^{viii}	3.525 (3)	O1···H2	3.052 (19)
F5···C1 ^v	3.532 (3)	N1···H2	2.37 (3)
F5···C1 ^{viii}	3.432 (3)	N2···H1	2.37 (3)
F5···C2 ^{viii}	3.466 (3)	C2···H1	2.61 (3)
F5···C13 ^{viii}	3.442 (3)	C6···H1	3.12 (3)
F6···F3 ⁱⁱ	3.0309 (19)	C8···H2	2.66 (3)
F6···F4 ⁱ	2.8319 (18)	C12···H2	3.13 (3)
F6···F4 ⁱⁱ	3.4627 (19)	H1···H2	2.13 (4)
F6···F7 ^{ix}	3.4730 (18)	F1···H1 ⁱⁱ	3.46 (3)
F6···C4 ⁱⁱ	3.162 (3)	F4···H2 ^{viii}	3.39 (3)
F6···C5 ⁱⁱ	3.377 (3)	F5···H1 ^v	2.60 (3)
F6···C10 ⁱⁱⁱ	3.395 (3)	F5···H1 ^{vi}	3.52 (3)
F6···C11 ⁱⁱⁱ	3.333 (3)	F10···H2 ^v	2.74 (3)
F6···C12 ⁱⁱⁱ	3.486 (3)	O1···H1 ^v	2.06 (2)
F7···F3 ^x	2.9024 (18)	O1···H2 ^v	2.01 (2)
F7···F6 ^{xi}	3.4730 (18)	C1···H1 ^v	3.460 (19)
F7···F7 ^{xi}	2.773 (2)	C6···H1 ^v	2.97 (3)
F7···F7 ^{ix}	2.773 (2)	C7···H2 ^v	3.44 (2)
F7···F8 ⁱⁱⁱ	3.208 (3)	C11···H2 ^v	3.60 (3)
F7···F8 ^{ix}	3.316 (2)	C12···H2 ^v	2.97 (3)
F7···C9 ^{ix}	3.246 (3)	C13···H1 ^v	3.160 (19)

F7···C10 ^{ix}	3.504 (3)	C13···H2 ^v	3.123 (19)
F8···F2 ^x	2.8148 (18)	H1···F1 ^{vi}	3.46 (3)
F8···F3 ^{xii}	3.131 (2)	H1···F5 ⁱⁱⁱ	2.60 (3)
F8···F3 ^x	3.119 (2)	H1···F5 ⁱⁱ	3.52 (3)
F8···F7 ^v	3.208 (3)	H1···O1 ⁱⁱⁱ	2.06 (2)
F8···F7 ^{xi}	3.316 (2)	H1···C1 ⁱⁱⁱ	3.460 (19)
F8···F9 ^{xiii}	3.026 (2)	H1···C6 ⁱⁱⁱ	2.97 (3)
F8···C9 ^v	3.568 (3)	H1···C13 ⁱⁱⁱ	3.160 (19)
F9···F2 ^{viii}	3.1594 (19)	H2···F4 ⁱ	3.39 (3)
F9···F8 ^{xiv}	3.026 (2)	H2···F10 ⁱⁱⁱ	2.74 (3)
F9···F9 ^{xiv}	3.1405 (19)	H2···O1 ⁱⁱⁱ	2.01 (2)
F9···F9 ^{xiii}	3.1405 (19)	H2···C7 ⁱⁱⁱ	3.44 (2)
F9···C7 ^v	3.448 (3)	H2···C11 ⁱⁱⁱ	3.60 (3)
F9···C8 ^v	3.356 (3)	H2···C12 ⁱⁱⁱ	2.97 (3)
F9···C9 ^v	3.487 (3)	H2···C13 ⁱⁱⁱ	3.123 (19)
F9···C10 ^{xiv}	3.133 (3)		
C1—N1—C13	124.23 (17)	F6—C8—C7	119.45 (16)
C7—N2—C13	122.57 (16)	F6—C8—C9	118.75 (17)
N1—C1—C2	118.94 (18)	C7—C8—C9	121.79 (19)
N1—C1—C6	123.82 (17)	F7—C9—C8	120.16 (19)
C2—C1—C6	117.09 (17)	F7—C9—C10	120.19 (17)
F1—C2—C1	119.10 (16)	C8—C9—C10	119.65 (18)
F1—C2—C3	118.66 (17)	F8—C10—C9	120.58 (18)
C1—C2—C3	122.19 (18)	F8—C10—C11	119.58 (19)
F2—C3—C2	119.74 (18)	C9—C10—C11	119.84 (17)
F2—C3—C4	120.90 (16)	F9—C11—C10	120.09 (17)
C2—C3—C4	119.36 (18)	F9—C11—C12	120.21 (17)
F3—C4—C3	120.55 (18)	C10—C11—C12	119.70 (19)
F3—C4—C5	119.96 (19)	F10—C12—C7	119.93 (16)
C3—C4—C5	119.49 (17)	F10—C12—C11	118.52 (18)
F4—C5—C4	119.68 (17)	C7—C12—C11	121.54 (18)
F4—C5—C6	119.63 (17)	O1—C13—N1	123.73 (17)
C4—C5—C6	120.70 (19)	O1—C13—N2	123.75 (17)
F5—C6—C1	120.90 (16)	N1—C13—N2	112.52 (17)
F5—C6—C5	118.00 (17)	C1—N1—H1	116.7 (17)
C1—C6—C5	121.09 (18)	C13—N1—H1	119.0 (17)
N2—C7—C8	120.58 (17)	C7—N2—H2	118.2 (17)
N2—C7—C12	121.92 (17)	C13—N2—H2	118.4 (17)
C8—C7—C12	117.45 (17)		
C1—N1—C13—O1	-3.5 (3)	F4—C5—C6—F5	2.1 (3)
C1—N1—C13—N2	177.01 (17)	F4—C5—C6—C1	-178.37 (15)
C13—N1—C1—C2	133.29 (19)	C4—C5—C6—F5	-177.65 (17)
C13—N1—C1—C6	-51.4 (3)	C4—C5—C6—C1	1.8 (3)
C7—N2—C13—O1	-0.5 (3)	N2—C7—C8—F6	0.8 (3)
C7—N2—C13—N1	179.00 (16)	N2—C7—C8—C9	-178.16 (16)
C13—N2—C7—C8	-125.94 (19)	N2—C7—C12—F10	0.4 (3)
C13—N2—C7—C12	56.8 (3)	N2—C7—C12—C11	179.16 (16)

N1—C1—C2—F1	−3.3 (3)	C8—C7—C12—F10	−176.99 (16)
N1—C1—C2—C3	174.14 (16)	C8—C7—C12—C11	1.8 (3)
N1—C1—C6—F5	3.0 (3)	C12—C7—C8—F6	178.23 (16)
N1—C1—C6—C5	−176.48 (16)	C12—C7—C8—C9	−0.8 (3)
C2—C1—C6—F5	178.43 (16)	F6—C8—C9—F7	−0.1 (3)
C2—C1—C6—C5	−1.1 (3)	F6—C8—C9—C10	179.98 (15)
C6—C1—C2—F1	−178.95 (16)	C7—C8—C9—F7	178.88 (17)
C6—C1—C2—C3	−1.5 (3)	C7—C8—C9—C10	−1.0 (3)
F1—C2—C3—F2	0.4 (3)	F7—C9—C10—F8	1.7 (3)
F1—C2—C3—C4	−179.26 (15)	F7—C9—C10—C11	−178.09 (17)
C1—C2—C3—F2	−177.03 (17)	C8—C9—C10—F8	−178.41 (18)
C1—C2—C3—C4	3.3 (3)	C8—C9—C10—C11	1.8 (3)
F2—C3—C4—F3	−1.5 (3)	F8—C10—C11—F9	−1.1 (3)
F2—C3—C4—C5	177.88 (16)	F8—C10—C11—C12	179.42 (16)
C2—C3—C4—F3	178.15 (17)	C9—C10—C11—F9	178.72 (18)
C2—C3—C4—C5	−2.5 (3)	C9—C10—C11—C12	−0.8 (3)
F3—C4—C5—F4	−0.4 (3)	F9—C11—C12—F10	−1.8 (3)
F3—C4—C5—C6	179.35 (16)	F9—C11—C12—C7	179.43 (16)
C3—C4—C5—F4	−179.83 (18)	C10—C11—C12—F10	177.76 (17)
C3—C4—C5—C6	−0.0 (3)	C10—C11—C12—C7	−1.0 (3)

Symmetry codes: (i) $-x+1, y+1/2, -z+1/2$; (ii) $-x+2, y+1/2, -z+1/2$; (iii) $x+1, y, z$; (iv) $-x+3/2, -y+1, z-1/2$; (v) $x-1, y, z$; (vi) $-x+2, y-1/2, -z+1/2$; (vii) $-x+1/2, -y+1, z-1/2$; (viii) $-x+1, y-1/2, -z+1/2$; (ix) $x+1/2, -y+3/2, -z+1$; (x) $-x+3/2, -y+1, z+1/2$; (xi) $x-1/2, -y+3/2, -z+1$; (xii) $-x+1/2, -y+1, z+1/2$; (xiii) $x+1/2, -y+1/2, -z+1$; (xiv) $x-1/2, -y+1/2, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
N1—H1 \cdots O1 ⁱⁱⁱ	0.864 (18)	2.057 (18)	2.850 (3)	152 (3)
N2—H2 \cdots O1 ⁱⁱⁱ	0.879 (18)	2.008 (18)	2.825 (3)	154 (3)

Symmetry code: (iii) $x+1, y, z$.